

Author index

- Allouche, A.R., see Magnier, S. 246 (1999) 57
- Amorim, J., J.L.S. Lino, J. Loureiro, M.A.P. Lima and F.J. da Paixão, Superelastic collisions of electrons with the $c^3\Pi_u$ metastable state in hydrogen dc positive column 246 (1999) 275
- Andrés, J., see Rotinov, A. 246 (1999) 1
- Aubert-Frécon, M., see Magnier, S. 246 (1999) 57
- Baumgarten, M., see Zhang, J. 246 (1999) 209
- Bens, A.T., see Ern, J. 246 (1999) 115
- Blau, W.J., see Holzer, W. 246 (1999) 445
- Bohr, H.G., K.J. Jalkanen, M. Elstner, K. Frimand and S. Suhai, A comparative study of MP2, B3LYP, RHF and SCC-DFTB force fields in predicting the vibrational spectra of N-acetyl-L-alanine-N'-methyl amide: VA and VCD spectra 246 (1999) 13
- Boilot, J.-P., see Brunel, M. 246 (1999) 477
- Bordat, P. and R. Brown, A molecular model of *p*-terphenyl and its disorder–order transition 246 (1999) 323
- Bradley, D.D.C., see Holzer, W. 246 (1999) 445
- Brown, R., see Bordat, P. 246 (1999) 323
- Brun, A., see Brunel, M. 246 (1999) 477
- Brunel, M., B. Campagne, M. Canva, A. Brun, F. Chaput and J.-P. Boilot, Ultrafast induced excited state absorption in organically doped xerogels 246 (1999) 477
- Caballero, N.B., E. Castellano, C.J. Cobos, A.E. Croce and G.A. Pino, Kinetics of the recombination reactions of CCIF with CF_2 and with CCIF 246 (1999) 157
- Campagne, B., see Brunel, M. 246 (1999) 477
- Canva, M., see Brunel, M. 246 (1999) 477
- Caputo, M.C., see Lazzeretti, P. 246 (1999) 75
- Castellano, E., see Caballero, N.B. 246 (1999) 157
- Catalán, J., see Palomar, J. 246 (1999) 167
- Cattaneo, P., M. Persico and A. Tani, Nonadiabatic processes in solution: molecular dynamics and surface hopping 246 (1999) 315
- Chaput, F., see Brunel, M. 246 (1999) 477
- Chuchani, G., see Rotinov, A. 246 (1999) 1
- Cobos, C.J., see Caballero, N.B. 246 (1999) 157
- Croce, A.E., see Caballero, N.B. 246 (1999) 157
- Curtiss, L.A., see Szarka, A.Z. 246 (1999) 147
- Da Paixão, F.J., see Amorim, J. 246 (1999) 275
- Decleva, P., see Fronzoni, G. 246 (1999) 127
- De Paz, J.L.G., see Palomar, J. 246 (1999) 167

- Dietz, F. and N. Tyutyulkov, Structure and properties of non-classical polymers. Part XII: A new family of high-spin polycyclic 1-D systems 246 (1999) 255
- Di Stefano, G., M. Lenzi and A. Ricci, Linestrengths of phosphorus monohydride. II. Isotope effect in the PX ($X = H, D$) $b\ ^1\Sigma^+ (v' = 0) \rightarrow X\ ^3\Sigma^- (v'' = 0)$ emission 246 (1999) 267
- Domingo, L.R., see Rotinov, A. 246 (1999) 1
- Elstner, M., see Bohr, H.G. 246 (1999) 13
- Ern, J., A.T. Bens, H.-D. Martin, S. Mukamel, D. Schmid, S. Tretiak, E. Tsiper and C. Krysch, Reaction dynamics of photochromic dithienylethene derivatives 246 (1999) 115
- Ferraro, M.B., see Lazzeretti, P. 246 (1999) 75
- Forés, M. and S. Scheiner, Effects of chemical substitution upon excited state proton transfer. Fluoroderivatives of salicylaldimine 246 (1999) 65
- Fratzl, P., see Mezei, R. 246 (1999) 295
- Frimand, K., see Bohr, H.G. 246 (1999) 13
- Fronzoni, G., M. Stener and P. Decleva, Theoretical description of the NEXAFS Cl 1s and 2p spectra of ClF and ClF₃ 246 (1999) 127
- Georges, R., see Herman, M. 246 (1999) 433
- Grozema, F.C., R.W.J. Zijlstra and P.Th. van Duijnen, Many-body interactions calculated with the direct reaction field model 246 (1999) 217
- Hadlinger, G., see Magnier, S. 246 (1999) 57
- Hadj Bachir, I., see Herman, M. 246 (1999) 433
- Haunert, G. and E. Tiemann, Total fragmentation of SbCl₃ by multiphoton dissociation in the UV 246 (1999) 381
- Havenith, R.W.A., H.J.J. van Dam, J.H. van Lenthe and L.W. Jenneskens, The excitation energies of 1,1'-bicyclohexylidene and 1,1':4',1''-tercyclohexylidene. A comparison of multi-reference configuration interaction and perturbation theory approaches 246 (1999) 49
- Hepp, M., see Herman, M. 246 (1999) 433
- Herman, M., F. Herregodts, R. Georges, M. Hepp, I. Hadj Bachir, M. Lecoutre and I. Kleiner, Spectroscopic investigation of vibration-rotation bands in acetaldehyde: Focus on the $n\nu_3$ ($n = 1-5$) aldehyde CH stretch bands 246 (1999) 433
- Herregodts, F., see Herman, M. 246 (1999) 433
- Holzer, W., M. Pichlmaier, A. Penzkofer, D.D.C. Bradley and W.J. Blau, Fluorescence spectroscopic behaviour of neat and blended conjugated polymer thin films 246 (1999) 445
- Huang, K.L., see Liou, H.T. 246 (1999) 391
- Hurst, J.K., P. Wormell, E. Krausz and A.R. Lacey, The electronic spectrum of 1, 4, 5, 8-tetraazaphthalene 246 (1999) 229
- Jalkanen, K.J., see Bohr, H.G. 246 (1999) 13
- Jenneskens, L.W., see Havenith, R.W.A. 246 (1999) 49
- Jordan, P.C., see Tanizaki, S. 246 (1999) 37
- Kim, J.H., see Lim, A.R. 246 (1999) 373
- Kleiner, I., see Herman, M. 246 (1999) 433
- Korth, O., A. Wiehe, H. Kurreck and B. Röder, Photoinduced intramolecular electron transfer in covalently linked porphyrin-triptycene-(bis)quinone diads and triads 246 (1999) 363

- Krausz, E., see Hurst, J.K. 246 (1999) 229
- Kryschi, C., see Ern, J. 246 (1999) 115
- Kurreck, H., see Korth, O. 246 (1999) 363
- Lacey, A.R., see Hurst, J.K. 246 (1999) 229
- Lazzeretti, P., M.C. Caputo and M.B. Ferraro, Thomas–Reiche–Kuhn populations in alkanes 246 (1999) 75
- Lecoutre, M., see Herman, M. 246 (1999) 433
- Lemaistre, J.P., Localization length and intraband scattering of excitons in linear aggregates 246 (1999) 283
- Lenzi, M., see Di Stefano, G. 246 (1999) 267
- Lim, A.R., J.H. Kim and B.M. Novak, Rigidity of the backbone for poly(bis(4-butoxy-carbonylphenyl))carbodiimide and poly(bis(4-butylphenyl))carbodiimide studied by solid state ^{13}C $T_{1\rho}$ measurements 246 (1999) 373
- Lima, M.A.P., see Amorim, J. 246 (1999) 275
- Lino, J.L.S., see Amorim, J. 246 (1999) 275
- Liou, H.T. and K.L. Huang, Fermi-resonances, potential energy function, and cluster-like spectra of the ground electronic state of CS_2 246 (1999) 391
- Lluch, J.M., see Paz, J.J. 246 (1999) 103
- Loureiro, J., see Amorim, J. 246 (1999) 275
- Magnier, S., S. Rousseau, A.R. Allouche, G. Hadinger and M. Aubert-Frécon, Potential energy curves of 58 states of Li_2^+ 246 (1999) 57
- Martin, H.-D., see Ern, J. 246 (1999) 115
- Mavri, J., see Tanizaki, S. 246 (1999) 37
- Mezei, R., K. Sinkó, J. Rohonczy, O. Paris and P. Fratzl, Short- and intermediate-range structure in Al(III)-containing gels prepared from Al-nitrate in organic medium 246 (1999) 295
- Miller, J.R., see Szarka, A.Z. 246 (1999) 147
- Mitra, S. and N. Tamai, A combined experimental and theoretical study on the photochromism of aromatic anils 246 (1999) 463
- Möller, S. and G. Weiser, Photoconductivity of polydiacetylene chains in polymer and monomer single crystals 246 (1999) 483
- Moreno, M., see Paz, J.J. 246 (1999) 103
- Msezane, A.Z., see Ozimba, P.A. 246 (1999) 87
- Mukamel, S., see Ern, J. 246 (1999) 115
- Novak, B.M., see Lim, A.R. 246 (1999) 373
- Ozimba, P.A. and A.Z. Msezane, Regge pole representation of the limiting behavior of optically forbidden transitions in atoms and molecules 246 (1999) 87
- Palomar, J., J.L.G. De Paz and J. Catalán, Vibrational study of intramolecular hydrogen bonding in *o*-hydroxybenzoyl compounds 246 (1999) 167
- Paris, O., see Mezei, R. 246 (1999) 295
- Partridge, H., see Tanizaki, S. 246 (1999) 37
- Paz, J.J., M. Moreno and J.M. Lluch, Effect of deuteration on the fluorescence excitation spectrum of tropolone: a theoretical study 246 (1999) 103
- Penzkofer, A., see Holzer, W. 246 (1999) 445
- Persico, M., see Cattaneo, P. 246 (1999) 315

- Pichlmaier, M., see Holzer, W. 246 (1999) 445
Pino, G.A., see Caballero, N.B. 246 (1999) 157
Popa-Nita, V., Magnetic-field-induced isotropic-nematic phase transition in porous media 246 (1999) 247
- Ricci, A., see Di Stefano, G. 246 (1999) 267
Röder, B., see Korth, O. 246 (1999) 363
Rohonczy, J., see Mezei, R. 246 (1999) 295
Rotinov, A., G. Chuchani, J. Andrés, L.R. Domingo and V.S. Safont, A combined experimental and theoretical study of the unimolecular elimination kinetics of 2-alkoxypropionic acids in the gas phase 246 (1999) 1
Rousseau, S., see Magnier, S. 246 (1999) 57
- Safont, V.S., see Rotinov, A. 246 (1999) 1
Scheiner, S., see Forés, M. 246 (1999) 65
Schmid, D., see Ern, J. 246 (1999) 115
Sinkó, K., see Mezei, R. 246 (1999) 295
Sohlberg, K., Mechanism of efficient V–V in collisions of $N_2^+(\nu > 0)$ with N_2 246 (1999) 307
Springborg, M., Dimensionality effects on the electronic and structural properties of PtS_2 chains 246 (1999) 347
Stener, M., see Fronzoni, G. 246 (1999) 127
Suhai, S., see Bohr, H.G. 246 (1999) 13
Szarka, A.Z., L.A. Curtiss and J.R. Miller, Calculation of temporary anion states using density functional theory 246 (1999) 147
Szorek, R., Dynamics of linear polymers in dilute solutions 246 (1999) 335
- Tamai, N., see Mitra, S. 246 (1999) 463
Tani, A., see Cattaneo, P. 246 (1999) 315
Tanizaki, S., J. Mavri, H. Partridge and P.C. Jordan, Unusual distributed charge models of water's electric potential 246 (1999) 37
Tiemann, E., see Haunert, G. 246 (1999) 381
Tretiak, S., see Ern, J. 246 (1999) 115
Tsiper, E., see Ern, J. 246 (1999) 115
Tyutyulkov, N., see Dietz, F. 246 (1999) 255
- Van Dam, H.J.J., see Havenith, R.W.A. 246 (1999) 49
Van Duijnen, P.Th., see Grozema, F.C. 246 (1999) 217
Van Lenthe, J.H., see Havenith, R.W.A. 246 (1999) 49
- Wang, L., see Zhang, J. 246 (1999) 209
Wang, R., see Zhang, J. 246 (1999) 209
Weiser, G., see Möller, S. 246 (1999) 483
Wiehe, A., see Korth, O. 246 (1999) 363
Wormell, P., see Hurst, J.K. 246 (1999) 229
- Zhang, J., R. Wang, L. Wang and M. Baumgarten, Using triazine as coupling unit for intramolecular ferromagnetic coupling of multiradicals 246 (1999) 209
Zijlstra, R.W.J., see Grozema, F.C. 246 (1999) 217

Subject index

Methods and constructs

Theoretical

Computational methods for electronic structure

- A combined experimental and theoretical study of the unimolecular elimination kinetics of 2-alkoxypropionic acids in the gas phase, A. Rotinov, G. Chuchani, J. Andrés, L.R. Domingo and V.S. Safont 246 (1999) 1
- A comparative study of MP2, B3LYP, RHF and SCC-DFTB force fields in predicting the vibrational spectra of N-acetyl-L-alanine-N'-methyl amide: VA and VCD spectra, H.G. Bohr, K.J. Jalkanen, M. Elstner, K. Frimand and S. Suhai 246 (1999) 13
- Unusual distributed charge models of water's electric potential, S. Tanizaki, J. Mavri, H. Partridge and P.C. Jordan 246 (1999) 37
- The excitation energies of 1,1'-bicyclohexylidene and 1,1':4',1''-tercyclohexylidene. A comparison of multi-reference configuration interaction and perturbation theory approaches, R.W.A. Havenith, H.J.J. van Dam, J.H. van Lenthe and L.W. Jenneskens 246 (1999) 49
- Potential energy curves of 58 states of Li_2^+ , S. Magnier, S. Rousseau, A.R. Allouche, G. Hadinger and M. Aubert-Frécon 246 (1999) 57
- Effects of chemical substitution upon excited state proton transfer. Fluoroderivatives of salicylaldimine, M. Forés and S. Scheiner 246 (1999) 65
- Thomas-Reiche-Kuhn populations in alkanes, P. Lazzeretti, M.C. Caputo and M.B. Ferraro 246 (1999) 75
- Regge pole representation of the limiting behavior of optically forbidden transitions in atoms and molecules, P.A. Ozimba and A.Z. Msezane 246 (1999) 87
- Effect of deuteration on the fluorescence excitation spectrum of tropolone: a theoretical study, J.J. Paz, M. Moreno and J.M. Lluch 246 (1999) 103
- Reaction dynamics of photochromic dithienylethene derivatives, J. Ern, A.T. Bens, H.-D. Martin, S. Mukamel, D. Schmid, S. Tretiak, E. Tsiper and C. Kryski 246 (1999) 115
- perturbative and many body approaches*
- Theoretical description of the NEXAFS Cl 1s and 2p spectra of ClF and ClF₃, G. Fronzoni, M. Stener and P. Decleva 246 (1999) 127
- density functional theory*
- Theoretical description of the NEXAFS Cl 1s and 2p spectra of ClF and ClF₃, G. Fronzoni, M. Stener and P. Decleva 246 (1999) 127

- Calculation of temporary anion states using density functional theory, A.Z. Szarka, L.A. Curtiss and J.R. Miller 246 (1999) 147
- Kinetics of the recombination reactions of CClF with CF₂ and with CClF, N.B. Caballero, E. Castellano, C.J. Cobos, A.E. Croce and G.A. Pino 246 (1999) 157
- Vibrational study of intramolecular hydrogen bonding in *o*-hydroxybenzoyl compounds, J. Palomar, J.L.G. De Paz and J. Catalán 246 (1999) 167
- Semiempirical methods*
- Using triazine as coupling unit for intramolecular ferromagnetic coupling of multiradicals, J. Zhang, R. Wang, L. Wang and M. Baumgarten 246 (1999) 209
- Many-body interactions calculated with the direct reaction field model, F.C. Grozema, R.W.J. Zijlstra and P.Th. van Duijnen 246 (1999) 217
- The electronic spectrum of 1, 4, 5, 8-tetraazanaphthalene, J.K. Hurst, P. Wormell, E. Krausz and A.R. Lacey 246 (1999) 229
- Wavefunctions for highly excited and unbound states*
- Potential energy curves of 58 states of Li₂⁺, S. Magnier, S. Rousseau, A.R. Allouche, G. Hadinger and M. Aubert-Frécon 246 (1999) 57
- Effects of chemical substitution upon excited state proton transfer. Fluoroderivatives of salicylaldehyde, M. Forés and S. Scheiner 246 (1999) 65
- Calculation of temporary anion states using density functional theory, A.Z. Szarka, L.A. Curtiss and J.R. Miller 246 (1999) 147
- Spin states and magnetic interactions*
- Using triazine as coupling unit for intramolecular ferromagnetic coupling of multiradicals, J. Zhang, R. Wang, L. Wang and M. Baumgarten 246 (1999) 209
- Magnetic-field-induced isotropic-nematic phase transition in porous media, V. Popa-Nita 246 (1999) 247
- Structure and properties of non-classical polymers. Part XII: A new family of high-spin polycyclic 1-D systems, F. Dietz and N. Tyutyulkov 246 (1999) 255
- Molecular response to external fields (incl. optical susceptibilities, dichroism, hyperpolarizabilities)*
- Thomas-Reiche-Kuhn populations in alkanes, P. Lazzeretti, M.C. Caputo and M.B. Ferraro 246 (1999) 75
- Radiative (incl. relativistic) effects on molecules and molecular processes*
- Linestrengths of phosphorus monohydride. II. Isotope effect in the PX (X = H, D) b ¹Σ⁺ (v' = 0) → X ³Σ⁻ (v'' = 0) emission, G. Di Stefano, M. Lenzi and A. Ricci 246 (1999) 267
- Scattering of waves and particles*
- Regge pole representation of the limiting behavior of optically forbidden transitions in atoms and molecules, P.A. Ozimba and A.Z. Msezane 246 (1999) 87
- Superelastic collisions of electrons with the c ³Π_u metastable state in hydrogen dc positive column, J. Amorim, J.L.S. Lino, J. Loureiro, M.A.P. Lima and F.J. da Paixão 246 (1999) 275
- Localization length and intraband scattering of excitons in linear aggregates, J.P. Lemaistre 246 (1999) 283
- Short- and intermediate-range structure in Al(III)-containing gels prepared from Al-nitrate in organic medium, R. Mezei, K. Sinkó, J. Rohonczy, O. Paris and P. Fratzl 246 (1999) 295

Collisional and reactive molecular dynamics with non-frictional forces

- Mechanism of efficient V–V in collisions of $N_2^+(\nu > 0)$ with N_2 , K. Sohlberg 246 (1999) 307

Intramolecular dynamics

- Effect of deuteration on the fluorescence excitation spectrum of tropolone: a theoretical study, J.J. Paz, M. Moreno and J.M. Lluch 246 (1999) 103

Molecular dynamics of many particle systems and condensed phases

- Many-body interactions calculated with the direct reaction field model, F.C. Grozema, R.W.J. Zijlstra and P.Th. van Duijnen 246 (1999) 217
- Nonadiabatic processes in solution: molecular dynamics and surface hopping, P. Cattaneo, M. Persico and A. Tani 246 (1999) 315
- A molecular model of *p*-terphenyl and its disorder–order transition, P. Bordat and R. Brown 246 (1999) 323

Statistical computational methods (incl. Monte Carlo)

- Kinetics of the recombination reactions of CCIF with CF_2 and with CCIF, N.B. Caballero, E. Castellano, C.J. Cobos, A.E. Croce and G.A. Pino 246 (1999) 157

Dynamics of structures, lattices and macromolecular conformations

- Dynamics of linear polymers in dilute solutions, R. Szorek 246 (1999) 335
- Dimensionality effects on the electronic and structural properties of PtS_2 chains, M. Springborg 246 (1999) 347
- Photoinduced intramolecular electron transfer in covalently linked porphyrin–tritycene–(bis)quinone diads and triads, O. Korth, A. Wiehe, H. Kurreck and B. Röder 246 (1999) 363

Fluctuations and random processes

- Localization length and intraband scattering of excitons in linear aggregates, J.P. Lemaistre 246 (1999) 283

Experiment*Magnetic resonances*

- Short- and intermediate-range structure in Al(III)-containing gels prepared from Al-nitrate in organic medium, R. Mezei, K. Sinkó, J. Rohonczy, O. Paris and P. Fratzl 246 (1999) 295
- Rigidity of the backbone for poly(bis(4-butoxycarbonylphenyl))carbodiimide and poly(bis(4-butylphenyl))carbodiimide studied by solid state ^{13}C $T_{1\rho}$ measurements, A.R. Lim, J.H. Kim and B.M. Novak 246 (1999) 373

Molecular spectroscopy

- The electronic spectrum of 1, 4, 5, 8-tetraazanaphthalene, J.K. Hurst, P. Wormell, E. Krausz and A.R. Lacey 246 (1999) 229
- Linestrengths of phosphorus monohydride. II. Isotope effect in the PX ($X = H, D$) $b\ ^1\Sigma^+$ ($v' = 0$) \rightarrow $X\ ^3\Sigma^-$ ($v'' = 0$) emission, G. Di Stefano, M. Lenzi and A. Ricci 246 (1999) 267
- Photoinduced intramolecular electron transfer in covalently linked porphyrin–tritycene–(bis)quinone diads and triads, O. Korth, A. Wiehe, H. Kurreck and B. Röder 246 (1999) 363
- Total fragmentation of $SbCl_3$ by multiphoton dissociation in the UV, G. Haunert and E. Tiemann 246 (1999) 381
- Fermi-resonances, potential energy function, and cluster-like spectra of the ground electronic state of CS_2 , H.T. Liou and K.L. Huang 246 (1999) 391

- Spectroscopic investigation of vibration–rotation bands in acetaldehyde: Focus on the $n\nu_3$ ($n = 1-5$) aldehyde CH stretch bands, M. Herman, F. Herregodts, R. Georges, M. Hepp, I. Hadj Bachir, M. Lecoutre and I. Kleiner 246 (1999) 433
- infrared*
- Vibrational study of intramolecular hydrogen bonding in *o*-hydroxybenzoyl compounds, J. Palomar, J.L.G. De Paz and J. Catalán 246 (1999) 167
- UV*
- The electronic spectrum of 1, 4, 5, 8-tetraazanaphthalene, J.K. Hurst, P. Wormell, E. Krausz and A.R. Lacey 246 (1999) 229
- visible*
- Linestrengths of phosphorus monohydride. II. Isotope effect in the PX ($X = H, D$) $b\ ^1\Sigma^+$ ($v' = 0$) \rightarrow $X\ ^3\Sigma^-$ ($v'' = 0$) emission, G. Di Stefano, M. Lenzi and A. Ricci 246 (1999) 267
- Fluorescence spectroscopic behaviour of neat and blended conjugated polymer thin films, W. Holzer, M. Pichlmaier, A. Penzkofer, D.D.C. Bradley and W.J. Blau 246 (1999) 445
- Laser induced fluorescence*
- Fermi-resonances, potential energy function, and cluster-like spectra of the ground electronic state of CS_2 , H.T. Liou and K.L. Huang 246 (1999) 391
- Ultrafast measurements*
- Reaction dynamics of photochromic dithienylethene derivatives, J. Ern, A.T. Bens, H.-D. Martin, S. Mukamel, D. Schmid, S. Tretiak, E. Tsiper and C. Kryschi 246 (1999) 115
- A combined experimental and theoretical study on the photochromism of aromatic anils, S. Mitra and N. Tamai 246 (1999) 463
- Ultrafast induced excited state absorption in organically doped xerogels, M. Brunel, B. Campagne, M. Canva, A. Brun, F. Chaput and J.-P. Boilot 246 (1999) 477
- Multiple resonance spectroscopy*
- Fermi-resonances, potential energy function, and cluster-like spectra of the ground electronic state of CS_2 , H.T. Liou and K.L. Huang 246 (1999) 391
- Optoacoustic spectroscopy*
- Spectroscopic investigation of vibration–rotation bands in acetaldehyde: Focus on the $n\nu_3$ ($n = 1-5$) aldehyde CH stretch bands, M. Herman, F. Herregodts, R. Georges, M. Hepp, I. Hadj Bachir, M. Lecoutre and I. Kleiner 246 (1999) 433
- Atomic and molecular beam techniques*
- Spectroscopic investigation of vibration–rotation bands in acetaldehyde: Focus on the $n\nu_3$ ($n = 1-5$) aldehyde CH stretch bands, M. Herman, F. Herregodts, R. Georges, M. Hepp, I. Hadj Bachir, M. Lecoutre and I. Kleiner 246 (1999) 433
- Small angle X-ray and neutron diffraction*
- Short- and intermediate-range structure in Al(III)-containing gels prepared from Al-nitrate in organic medium, R. Mezei, K. Sinkó, J. Rohonczy, O. Paris and P. Fratzl 246 (1999) 295

Measurement of macroscopic variables

- Kinetics of the recombination reactions of CClF with CF₂ and with CClF, N.B. Caballero, E. Castellano, C.J. Cobos, A.E. Croce and G.A. Pino 246 (1999) 157
- Photoconductivity of polydiacetylene chains in polymer and monomer single crystals, S. Möller and G. Weiser 246 (1999) 483

Objects**Bulk systems***Gases*

- A combined experimental and theoretical study of the unimolecular elimination kinetics of 2-alkoxypropionic acids in the gas phase, A. Rotinov, G. Chuchani, J. Andrés, L.R. Domingo and V.S. Safont 246 (1999) 1
- Kinetics of the recombination reactions of CClF with CF₂ and with CClF, N.B. Caballero, E. Castellano, C.J. Cobos, A.E. Croce and G.A. Pino 246 (1999) 157
- Linestrengths of phosphorus monohydride. II. Isotope effect in the PX (X = H, D) b ¹Σ⁺ (v' = 0) → X ³Σ⁻ (v'' = 0) emission, G. Di Stefano, M. Lenzi and A. Ricci 246 (1999) 267

Liquid mixtures and solutions

- Reaction dynamics of photochromic dithienylethene derivatives, J. Ern, A.T. Bens, H.-D. Martin, S. Mukamel, D. Schmid, S. Tretiak, E. Tsiper and C. Kryschi 246 (1999) 115
- Nonadiabatic processes in solution: molecular dynamics and surface hopping, P. Cattaneo, M. Persico and A. Tani 246 (1999) 315
- Dynamics of linear polymers in dilute solutions, R. Szorek 246 (1999) 335
- Photoinduced intramolecular electron transfer in covalently linked porphyrin–tritycene–(bis)quinone diads and triads, O. Korth, A. Wiehe, H. Kurreck and B. Röder 246 (1999) 363
- A combined experimental and theoretical study on the photochromism of aromatic anils, S. Mitra and N. Tamai 246 (1999) 463

Crystals

- Photoconductivity of polydiacetylene chains in polymer and monomer single crystals, S. Möller and G. Weiser 246 (1999) 483

-neat

- A molecular model of *p*-terphenyl and its disorder–order transition, P. Bordat and R. Brown 246 (1999) 323

Complex fluids

- Magnetic-field-induced isotropic-nematic phase transition in porous media, V. Popa-Nita 246 (1999) 247

Polymers

- Structure and properties of non-classical polymers. Part XII: A new family of high-spin polycyclic 1-D systems, F. Dietz and N. Tyutyulkov 246 (1999) 255
- Dynamics of linear polymers in dilute solutions, R. Szorek 246 (1999) 335

- Rigidity of the backbone for poly(bis(4-butoxycarbonylphenyl))carbodiimide and poly(bis(4-butylphenyl))carbodiimide studied by solid state ^{13}C $T_{1\rho}$ measurements, A.R. Lim, J.H. Kim and B.M. Novak 246 (1999) 373
- Fluorescence spectroscopic behaviour of neat and blended conjugated polymer thin films, W. Holzer, M. Pichlmaier, A. Penzkofer, D.D.C. Bradley and W.J. Blau 246 (1999) 445
- Photoconductivity of polydiacetylene chains in polymer and monomer single crystals, S. Möller and G. Weiser 246 (1999) 483
- Thin films*
- Fluorescence spectroscopic behaviour of neat and blended conjugated polymer thin films, W. Holzer, M. Pichlmaier, A. Penzkofer, D.D.C. Bradley and W.J. Blau 246 (1999) 445
- Plasmas*
- Superelastic collisions of electrons with the $c^3\Pi_u$ metastable state in hydrogen dc positive column, J. Amorim, J.L.S. Lino, J. Loureiro, M.A.P. Lima and F.J. da Paixão 246 (1999) 275
- Microscopic and mesoscopic systems**
- Single atoms, molecules and assemblies (incl. biological)*
- Unusual distributed charge models of water's electric potential, S. Tanizaki, J. Mavri, H. Partridge and P.C. Jordan 246 (1999) 37
- Regge pole representation of the limiting behavior of optically forbidden transitions in atoms and molecules, P.A. Ozimba and A.Z. Msezane 246 (1999) 87
- Photoinduced intramolecular electron transfer in covalently linked porphyrin–tritycene–(bis)quinone diads and triads, O. Korth, A. Wiehe, H. Kurreck and B. Röder 246 (1999) 363
- Molecules (neutral and ionic)*
- A combined experimental and theoretical study of the unimolecular elimination kinetics of 2-alkoxypropionic acids in the gas phase, A. Rotinov, G. Chuchani, J. Andrés, L.R. Domingo and V.S. Safont 246 (1999) 1
- A comparative study of MP2, B3LYP, RHF and SCC-DFTB force fields in predicting the vibrational spectra of N-acetyl-L-alanine-N'-methyl amide: VA and VCD spectra, H.G. Bohr, K.J. Jalkanen, M. Elstner, K. Frimand and S. Suhai 246 (1999) 13
- The excitation energies of 1,1'-bicyclohexylidene and 1,1':4',1''-tercyclohexylidene. A comparison of multi-reference configuration interaction and perturbation theory approaches, R.W.A. Havenith, H.J.J. van Dam, J.H. van Lenthe and L.W. Jenneskens 246 (1999) 49
- Thomas–Reiche–Kuhn populations in alkanes, P. Lazzeretti, M.C. Caputo and M.B. Ferraro 246 (1999) 75
- Theoretical description of the NEXAFS Cl 1s and 2p spectra of ClF and ClF₃, G. Fronzoni, M. Stener and P. Decleva 246 (1999) 127
- Vibrational study of intramolecular hydrogen bonding in *o*-hydroxybenzoyl compounds, J. Palomar, J.L.G. De Paz and J. Catalán 246 (1999) 167
- Using triazine as coupling unit for intramolecular ferromagnetic coupling of multiradicals, J. Zhang, R. Wang, L. Wang and M. Baumgarten 246 (1999) 209
- Mechanism of efficient V–V in collisions of $\text{N}_2^+(\nu > 0)$ with N_2 , K. Sohlberg 246 (1999) 307
- Dimensionality effects on the electronic and structural properties of PtS₂ chains, M. Springborg 246 (1999) 347
- Fermi-resonances, potential energy function, and cluster-like spectra of the ground electronic state of CS₂, H.T. Liou and K.L. Huang 246 (1999) 391

- Ultrafast induced excited state absorption in organically doped xerogels, M. Brunel, B. Campagne, M. Canva, A. Brun, F. Chaput and J.-P. Boilot 246 (1999) 477
- Thomas–Reiche–Kuhn populations in alkanes, P. Lazzeretti, M.C. Caputo and M.B. Ferraro 246 (1999) 75
- diatomic*
- Potential energy curves of 58 states of Li_2^+ , S. Magnier, S. Rousseau, A.R. Allouche, G. Hadinger and M. Aubert-Frécon 246 (1999) 57
- Superelastic collisions of electrons with the $c^3\Pi_u$ metastable state in hydrogen dc positive column, J. Amorim, J.L.S. Lino, J. Loureiro, M.A.P. Lima and F.J. da Paixão 246 (1999) 275
- small polyatomics*
- Unusual distributed charge models of water's electric potential, S. Tanizaki, J. Mavri, H. Partridge and P.C. Jordan 246 (1999) 37
- Effect of deuteration on the fluorescence excitation spectrum of tropolone: a theoretical study, J.J. Paz, M. Moreno and J.M. Lluch 246 (1999) 103
- Theoretical description of the NEXAFS Cl 1s and 2p spectra of ClF and ClF₃, G. Fronzoni, M. Stener and P. Decleva 246 (1999) 127
- Total fragmentation of SbCl₃ by multiphoton dissociation in the UV, G. Haunert and E. Tiemann 246 (1999) 381
- Spectroscopic investigation of vibration–rotation bands in acetaldehyde: Focus on the $n\nu_3$ ($n = 1-5$) aldehyde CH stretch bands, M. Herman, F. Herregodts, R. Georges, M. Hepp, I. Hadj Bachir, M. Lecoutre and I. Kleiner 246 (1999) 433
- aromatics*
- Effects of chemical substitution upon excited state proton transfer. Fluoroderivatives of salicylaldehyde, M. Forés and S. Scheiner 246 (1999) 65
- The electronic spectrum of 1, 4, 5, 8-tetraazaphthalene, J.K. Hurst, P. Wormell, E. Krausz and A.R. Lacey 246 (1999) 229
- A combined experimental and theoretical study on the photochromism of aromatic anils, S. Mitra and N. Tamai 246 (1999) 463
- other large*
- Reaction dynamics of photochromic dithienylethene derivatives, J. Ern, A.T. Bens, H.-D. Martin, S. Mukamel, D. Schmid, S. Tretiak, E. Tsiper and C. Kryschik 246 (1999) 115
- polymeric and biological*
- Fluorescence spectroscopic behaviour of neat and blended conjugated polymer thin films, W. Holzer, M. Pichlmaier, A. Penzkofer, D.D.C. Bradley and W.J. Blau 246 (1999) 445
- Molecular aggregates*
- Localization length and intraband scattering of excitons in linear aggregates, J.P. Lemaistre 246 (1999) 283
- clusters*
- Many-body interactions calculated with the direct reaction field model, F.C. Grozema, R.W.J. Zijlstra and P.Th. van Duijnen 246 (1999) 217

Free radicals (incl. hydronium and muonium)

- Kinetics of the recombination reactions of CCIF with CF₂ and with CCIF, N.B. Caballero, E. Castellano, C.J. Cobos, A.E. Croce and G.A. Pino 246 (1999) 157
- Using triazine as coupling unit for intramolecular ferromagnetic coupling of multiradicals, J. Zhang, R. Wang, L. Wang and M. Baumgarten 246 (1999) 209

Quasiparticles (incl. excitons)

- Localization length and intraband scattering of excitons in linear aggregates, J.P. Lemaistre 246 (1999) 283

Ions and charge carriers

- Calculation of temporary anion states using density functional theory, A.Z. Szarka, L.A. Curtiss and J.R. Miller 246 (1999) 147

Supramolecular assemblies (incl. nanoparticles and nanostructures)

- Short- and intermediate-range structure in Al(III)-containing gels prepared from Al-nitrate in organic medium, R. Mezei, K. Sinkó, J. Rohonczy, O. Paris and P. Fratzl 246 (1999) 295

Phenomena*Molecular structure*

- Rigidity of the backbone for poly(bis(4-butoxycarbonylphenyl))carbodiimide and poly(bis(4-butylphenyl))carbodiimide studied by solid state ¹³C T_{1ρ} measurements, A.R. Lim, J.H. Kim and B.M. Novak 246 (1999) 373

Vibrations and rotations of molecules

- Effect of deuteration on the fluorescence excitation spectrum of tropolone: a theoretical study, J.J. Paz, M. Moreno and J.M. Lluch 246 (1999) 103
- A molecular model of *p*-terphenyl and its disorder–order transition, P. Bordat and R. Brown 246 (1999) 323
- Rigidity of the backbone for poly(bis(4-butoxycarbonylphenyl))carbodiimide and poly(bis(4-butylphenyl))carbodiimide studied by solid state ¹³C T_{1ρ} measurements, A.R. Lim, J.H. Kim and B.M. Novak 246 (1999) 373
- Spectroscopic investigation of vibration–rotation bands in acetaldehyde: Focus on the *nν*₃ (*n* = 1–5) aldehyde CH stretch bands, M. Herman, F. Herregodts, R. Georges, M. Hepp, I. Hadj Bachir, M. Lecoutre and I. Kleiner 246 (1999) 433

Electronic structure and states

- Unusual distributed charge models of water's electric potential, S. Tanizaki, J. Mavri, H. Partridge and P.C. Jordan 246 (1999) 37
- The excitation energies of 1,1'-bicyclohexylidene and 1,1':4',1''-tercyclohexylidene. A comparison of multi-reference configuration interaction and perturbation theory approaches, R.W.A. Havenith, H.J.J. van Dam, J.H. van Lenthe and L.W. Jenneskens 246 (1999) 49
- Potential energy curves of 58 states of Li₂⁺, S. Magnier, S. Rousseau, A.R. Allouche, G. Hadinger and M. Aubert-Frécon 246 (1999) 57
- Calculation of temporary anion states using density functional theory, A.Z. Szarka, L.A. Curtiss and J.R. Miller 246 (1999) 147

- The electronic spectrum of 1, 4, 5, 8-tetraazanaphthalene, J.K. Hurst, P. Wormell, E. Krausz and A.R. Lacey 246 (1999) 229
- Fermi-resonances, potential energy function, and cluster-like spectra of the ground electronic state of CS₂, H.T. Liou and K.L. Huang 246 (1999) 391
- Photoconductivity of polydiacetylene chains in polymer and monomer single crystals, S. Möller and G. Weiser 246 (1999) 483
- Spin splittings*
- Using triazine as coupling unit for intramolecular ferromagnetic coupling of multiradicals, J. Zhang, R. Wang, L. Wang and M. Baumgarten 246 (1999) 209
- Molecular interactions*
- Regge pole representation of the limiting behavior of optically forbidden transitions in atoms and molecules, P.A. Ozimba and A.Z. Msezane 246 (1999) 87
- A molecular model of *p*-terphenyl and its disorder–order transition, P. Bordat and R. Brown 246 (1999) 323
- Energy transfer processes*
- Superelastic collisions of electrons with the c ³Π_u metastable state in hydrogen dc positive column, J. Amorim, J.L.S. Lino, J. Loureiro, M.A.P. Lima and F.J. da Paixão 246 (1999) 275
- Superelastic collisions of electrons with the c ³Π_u metastable state in hydrogen dc positive column, J. Amorim, J.L.S. Lino, J. Loureiro, M.A.P. Lima and F.J. da Paixão 246 (1999) 275
- Localization length and intraband scattering of excitons in linear aggregates, J.P. Lemaistre 246 (1999) 283
- Molecular photophysical processes*
- Linestrengths of phosphorus monohydride. II. Isotope effect in the PX (X = H, D) b ¹Σ⁺ (v' = 0) → X ³Σ⁻ (v'' = 0) emission, G. Di Stefano, M. Lenzi and A. Ricci 246 (1999) 267
- Photoinduced intramolecular electron transfer in covalently linked porphyrin–tritycene–(bis)quinone diads and triads, O. Korth, A. Wiehe, H. Kurreck and B. Röder 246 (1999) 363
- Photochemistry*
- Reaction dynamics of photochromic dithienylethene derivatives, J. Ern, A.T. Bens, H.-D. Martin, S. Mukamel, D. Schmid, S. Tretiak, E. Tsiper and C. Kryschi 246 (1999) 115
- Kinetics of the recombination reactions of CClF with CF₂ and with CClF, N.B. Caballero, E. Castellano, C.J. Cobos, A.E. Croce and G.A. Pino 246 (1999) 157
- Nonadiabatic processes in solution: molecular dynamics and surface hopping, P. Cattaneo, M. Persico and A. Tani 246 (1999) 315
- Total fragmentation of SbCl₃ by multiphoton dissociation in the UV, G. Haunert and E. Tiemann 246 (1999) 381
- A combined experimental and theoretical study on the photochromism of aromatic anils, S. Mitra and N. Tamai 246 (1999) 463
- Luminescence spectra, yields and lifetimes*
- Fluorescence spectroscopic behaviour of neat and blended conjugated polymer thin films, W. Holzer, M. Pichlmaier, A. Penzkofer, D.D.C. Bradley and W.J. Blau 246 (1999) 445
- Multiphoton phenomena*
- Total fragmentation of SbCl₃ by multiphoton dissociation in the UV, G. Haunert and E. Tiemann 246 (1999) 381

Reactions (incl. dissociation)

- A combined experimental and theoretical study of the unimolecular elimination kinetics of 2-alkoxypropionic acids in the gas phase, A. Rotinov, G. Chuchani, J. Andrés, L.R. Domingo and V.S. Safont 246 (1999) 1

-collisional

- Regge pole representation of the limiting behavior of optically forbidden transitions in atoms and molecules, P.A. Ozimba and A.Z. Msezane 246 (1999) 87

-condensed phase

- Vibrational study of intramolecular hydrogen bonding in *o*-hydroxybenzoyl compounds, J. Palomar, J.L.G. De Paz and J. Catalán 246 (1999) 167

Proton and hydrogen atom transfer

- Effects of chemical substitution upon excited state proton transfer. Fluoroderivatives of salicylaldehyde, M. Forés and S. Scheiner 246 (1999) 65
- A combined experimental and theoretical study on the photochromism of aromatic anils, S. Mitra and N. Tamai 246 (1999) 463

Ionization (incl. Rydberg states)

- Theoretical description of the NEXAFS Cl 1s and 2p spectra of ClF and ClF₃, G. Fronzoni, M. Stener and P. Decleva 246 (1999) 127

Surface chemical physics

- Fermi-resonances, potential energy function, and cluster-like spectra of the ground electronic state of CS₂, H.T. Liou and K.L. Huang 246 (1999) 391

-surface scattering

- Reaction dynamics of photochromic dithienylethene derivatives, J. Ern, A.T. Bens, H.-D. Martin, S. Mukamel, D. Schmid, S. Tretiak, E. Tsiper and C. Kryschi 246 (1999) 115
- A combined experimental and theoretical study on the photochromism of aromatic anils, S. Mitra and N. Tamai 246 (1999) 463

-surface reactions

- Fermi-resonances, potential energy function, and cluster-like spectra of the ground electronic state of CS₂, H.T. Liou and K.L. Huang 246 (1999) 391

-catalysis

- Spectroscopic investigation of vibration-rotation bands in acetaldehyde: Focus on the $n\nu_3$ ($n = 1-5$) aldehyde CH stretch bands, M. Herman, F. Herregodts, R. Georges, M. Hepp, I. Hadj Bachir, M. Lecoutre and I. Kleiner 246 (1999) 433

Electronic process in gases

- Superelastic collisions of electrons with the $c^3\Pi_u$ metastable state in hydrogen dc positive column, J. Amorim, J.L.S. Lino, J. Loureiro, M.A.P. Lima and F.J. da Paixão 246 (1999) 275
- Spectroscopic investigation of vibration-rotation bands in acetaldehyde: Focus on the $n\nu_3$ ($n = 1-5$) aldehyde CH stretch bands, M. Herman, F. Herregodts, R. Georges, M. Hepp, I. Hadj Bachir, M. Lecoutre and I. Kleiner 246 (1999) 433

Structure of solids, liquids and glasses

- Short- and intermediate-range structure in Al(III)-containing gels prepared from Al-nitrate in organic medium, R. Mezei, K. Sinkó, J. Rohonczy, O. Paris and P. Fratzl 246 (1999) 295

Critical behavior and phase transitions

- A molecular model of *p*-terphenyl and its disorder–order transition, P. Bordat and R. Brown 246 (1999) 323